

MULTIVARIATE DATA ANALYSIS METHOD AND USES THEREOF

RELATED APPLICATIONS

This application is a continuation-in-part of U.S. Patent Application Serial No. 10/293,092 filed November 13, 2002, which claims priority of U.S. Provisional Patent Application Serial No. 60/338,574 filed November 13, 2001. These applications are incorporated herein by reference.

BACKGROUND OF THE INVENTION

Design of a good information system based on several characteristics is an important requirement for successfully carrying out any decision-making activity. In many cases though a significant amount of information is available, we fail to use such information in a meaningful way. As we require high quality products in day-to-day life, it is also required to have high quality information systems to make robust decisions or predictions. To produce high quality products, it is well established that the variability in the processes must be reduced first. Variability can be accurately measured and reduced only if we have a suitable measurement system with appropriate measures. Similarly, in the design of information systems, it is essential to develop a measurement scale and use appropriate measures to make accurate predictions or decisions.

Usually, information systems deal with multidimensional characteristics. A multidimensional system could be an inspection system, a medical diagnosis system, a sensor system, a face/voice recognition system (any pattern recognition system), credit card/loan approval system, a weather forecasting

system or a university admission system. As we encounter these multidimensional systems in day-to-day life, it is important to have a measurement scale by which degree of abnormality (severity) can be measured to take appropriate decisions. In the case of medical diagnosis, the degree of abnormality refers to the severity of diseases and in the case of credit card/loan approval system it refers to the ability to pay back the balance/loan. If we have a measurement scale based on the characteristics of multidimensional systems, it greatly enhances the decision maker's ability to take judicious decisions. While developing a multidimensional measurement scale, it is essential to keep in mind the following criteria: 1) having a base or reference point to the scale, 2) validation of the scale, and 3) selection of useful subset of variables with suitable measures for future use.

There are several multivariate methods. These methods are being used in multidimensional applications, but still there are incidences of false alarms in applications like weather forecasting, airbag sensor operation, and medical diagnosis. These problems could be because of not having an adequate measurement system with suitable measures to determine or predict the degree of severity accurately.

SUMMARY OF THE INVENTION

A process for multivariate data analysis includes the steps of using an adjoint matrix to compute a new distance for a data set in a Mahalanobis space. The relation of a datum relative to the Mahalanobis space is then determined.

A medical diagnosis process includes defining a set of variables relating to a patient condition and collecting a data set of the set of variables for a normal group. Standardized values of the set of variables of the normal group are then computed and used to construct a Mahalanobis space. A distance for
5 an abnormal value outside the Mahalanobis space is then computed. Important variables from the set of variables are identified based on orthogonal arrays and signal to noise ratios. Subsequent monitoring of conditions occurs based upon the important variables.

BRIEF DESCRIPTION OF THE DRAWINGS

10 Figure 1 is a schematic illustrating a multi-dimensional diagnosis system of the present invention;

Figure 2 is a graphical representation of a voice recognition pattern according to the present invention parsed into the letter k subsets that correspond to k patterns numbered from 1,2,..k where each pattern starts at a
15 low value, reaches a maximum and then again returns to the low value;

Figure 3 is a graphical representation of MDAs values for normal and abnormal values for nine separate data points;

Figure 4 is a graphical representation of MDA values for normal versus abnormal values with important variable usage, for the data of Figure 3;

20 Figure 5 is a graphical representation of Gram-Schmidt predicted values as a function of variable number compared with assigned values for a seventeen variable test set; and

Figure 6 is a graphical representation of Gram-Schmidt predicted values as a function of variable number compared with assigned values for a nineteen variable test set including two variables with zero standard deviation.

DETAILED DESCRIPTION OF THE INVENTION

5 The inventive method helps develop multidimensional measurement scale by integrating mathematical and statistical concepts such as Mahalanobis distance and Gram-Schmidt's orthogonalization method, with the principles of quality engineering or Taguchi Methods.

10 The selection of unit group (Mahalanobis group) is the most important aspect of MTS and its related methods. Every individual observation in this group has a unique pattern. Since the conditions of the observations are measured from this group, it is desirable that observations within this group be as uniform as possible. From this group, the distances (of observations outside of this group) are measured to perform the diagnosis. These distances, which
15 are similar to the Mahalanobis distance, indicate the degree of severities of individual observations. A group of observations is needed (as in the case of the reference group) to measure distances because with one observation a correlation structure cannot be obtained. It should be noted that the correlation matrix corresponding to this reference group is also used to measure distances
20 outside of this group. In MTS, S/N ratios are calculated based on the observations that are outside of the unit space.

 In MTS and its related methods, the diagnosis is performed after validating the scale with variables defining the multidimensional system. The

validation is done with observations outside of unit group by computing S/N ratios. S/N ratio is the measure of correlation between “input signal” and “output” of the system. If there is a good correlation (higher S/N ratio), then the scale is useful for diagnosis.

5 One of the main objectives of the present invention is to introduce a scale based on all input characteristics to measure the degree of abnormality. In the case of medical diagnosis, for example, the aim is to measure the degree of severity of each disease based on this scale. To construct such a scale, Mahalanobis distance (MD) is used. MD is a squared distance (also denoted as
10 D^2) and is calculated for j^{th} observation, in a sample of size n with k variables, by using the following formula:

$$MD_j = D_j^2 = (1/k) Z_{ij} C^{-1} Z'_{ij} \quad (1)$$

Where,
15 $j = 1 \text{ to } n$
 $Z_{ij} = (z_{1j}, z_{2j}, \dots, z_{kj})$
 = standardized vector obtained by standardized values of X_{ij}
 ($i = 1..k$)
 $Z_{ij} = (X_{ij} - m_i) / s_i$
 X_{ij} = value of i^{th} characteristic in j^{th} observation
 m_i = mean of i^{th} characteristic
20 s_i = s.d. of i^{th} characteristic
 k = number of characteristics/variables
 $'$ = transpose of the vector
 C^{-1} = inverse of the correlation matrix

There is also an alternate way to compute MD values using Gram-
25 Schmidt's orthogonalization process. It can be seen that MD in Equation (1) is obtained by scaling, that is by dividing with k , the original Mahalanobis distance. MD can be considered as the mean square deviation (MSD) in multidimensional spaces. The present invention focuses on constructing a

normal group, or in the application of medical diagnosis a healthy group, from a data population, called Mahalanobis Space (MS). Defining the normal group or MS is the choice of a specialist conducting the data analysis. In case of medical diagnosis, the MS is constructed only for the people who are healthy
5 and in case of manufacturing inspection system, the MS is constructed for high quality products. Thus, MS is a database for the normal group consisting of the following quantities:

10 m_i = mean vector
 s_i = standard deviation vector
C= correlation matrix.

Since MD values are used to define the normal group, this group is designated as the Mahalanobis Space. It can be easily shown, with standardized values, that MS has zero point as the mean vector and the average MD as unity. Because the average MD of MS is unity, MS is also called as the
15 unit space. The zero point and the unit distance are used as reference point for the scale of normalcy relating to inclusion of a subject within MS. This scale is often operative in identifying the conditions outside the Mahalanobis Space. In order to validate the accuracy of the scale, different kinds of known conditions outside MS are used. If the scale is good, these conditions should have MDs
20 that match with decision maker's judgment. In this application, the conditions outside MS are not considered as a separate group (population) because the occurrence of these conditions are unique, for example a patient may be abnormal because of high blood pressure or because of high sugar content. Because of this reason, the same correlation matrix of the MS is used to

compute the MD values of each abnormal. MD of an abnormal point is the distance of that point from the center point of MS.

In the next phase of the invention, orthogonal arrays (OAs) and signal-to-noise (S/N) ratios are used to choose the relevant variables. There are
5 different kinds of S/N ratios depending on the prior knowledge about the severity of the abnormals.

A typical multidimensional system used in the present invention is as shown in Figure 1, where X_1, X_2, \dots, X_n correspond to the variables that provide a set of information to make a decision. Using these variables, MS is
10 constructed for the healthy or normal group, which becomes the reference point for the measurement scale. After constructing the MS, the measurement scale is validated by considering the conditions outside MS. These outside conditions are typically checked with the given input signals and in the presence of noise factors (if any). If the noise factors are present, a correct
15 decision has to be made about the state of the system. In the context of multivariate diagnosis system, it would be appropriate to consider two types of noise conditions. They are 1) active noise and 2) criminal noise. Example for active noise condition is change in usage environment such as conditions in different manufacturing environments or different hospitals and the example
20 for criminal noise conditions are unexpected conditions such as terrorist attacks on 11 September 2001 in which the system is operating. It is important to design multivariate information systems considering these two types of noise conditions. In Figure 1, the input signal is the true value of the state of the

system, if known. The output (MD) should have a good correlation with the true state of the system (input signal).. In most applications, it is not easy to obtain the true states of the system. In such cases, the working averages of the different classes, where the classes correspond to the different degrees of severity, can be considered as the input signals.

After validating the measurement scale, OAs and S/N ratios are used to identify the variables of importance. OAs are used to minimize the number of variable combinations to be tested. The variables are allocated to the columns of the array. In MTS analysis only two level OAs are used as there are only two levels for the variables – presence and absence.. To identify the variables of importance, S/N ratios are used.

The inventive process can illustratively be applied to a multidimensional system in four stages. The steps in each exemplary stage are listed below:

Stage I: Construction of a Measurement Scale with Mahalanobis Space (Unit Space) as the Reference

- Define the variables that determine the healthiness of a condition. For example, in medical diagnosis application, the doctor has to consider the variables of all diseases to define a healthy group. In general, for pattern recognition applications, the term “healthiness” must be defined with respect to “reference pattern”.
- Collect the data on all the variables from the healthy group.
- Compute the standardized values of the variables of the healthy group.

- Compute MDs of all observations. With these MDs, the zero point and the unit distance are defined.
- Use the zero point and the unit distance as the reference point or base for the measurement scale.

5 **Stage II: Validation of the Measurement Scale**

- Identify the abnormal conditions. In medical diagnosis applications, the abnormal conditions refer to the patients having different kinds of diseases. In fact, to validate the scale, any condition outside MS is chosen.
- Compute the MDs corresponding to these abnormal conditions to validate
10 the scale. The variables in the abnormal conditions are normalized by using the mean and s.d.s of the corresponding variables in the healthy group. The correlation matrix or set of Gram-Schmidt's coefficients, if Gram-Schmidt's method is used, corresponding to the healthy group is used for finding the MDs of abnormal conditions.
- If the scale is good, the MDs corresponding to the abnormal conditions
15 should have higher values. In this way the scale is validated. In other words, the MDs of conditions outside MS must match with judgment.

Stage III: Identify the Useful Variables (Developing Stage)

- Find out the useful set of variables using orthogonal arrays (OAs) and S/N
20 ratios. S/N ratio, obtained from the abnormal MDs, is used as the response for each combination of OA. The useful set of variables is obtained by evaluating the "gain" in S/N ratio.

Stage IV: Future Diagnosis with Useful Variables

Monitor the conditions using the scale, which is developed with the help of the useful set of variables. Based on the values of MDs, appropriate corrective actions can be taken. The decision to take the necessary actions depends on the value of the threshold.

In case of medical diagnosis application, above steps have to be performed for each kind of disease in the subsequent phases of diagnosis. It is appreciated that many additional applications for the present invention exist as illustratively recited in “The Mahalanobis Taguchi Strategy – A Pattern Technology System” by G. Taguchi and R. Jugulum, John-Wiley, 2002 and in “The Mahalanobis Taguchi System” by G. Taguchi et al., McGraw-Hill, 2001.

According to the present invention, an adjoint matrix method is used to calculate MD values.

If A is a square matrix, the inverse can be computed for square matrices only, then its inverse A^{-1} is given as:

$$A^{-1} = (1/\det. A) A_{adj} \quad (2)$$

Where,

A_{adj} is called adjoint matrix of A. Adjoint matrix is transpose of cofactor matrix, which is obtained by cofactors of all the elements of matrix A,

$\det. A$ is called determinant of the matrix A. The determinant is a characteristic number (scalar) associated with a square matrix. A matrix is said to be singular if its determinant is zero.

As mentioned before, the determinant is a characteristic number associated with a square matrix. The importance of determinant can be realized when solving a system of linear equations using matrix algebra. The solution to the system of equations contains inverse matrix term, which is
5 obtained by dividing the adjoint matrix by determinant. If the determinant is zero then, the solution does not exist.

Considering a 2 x 2 matrix as shown below:

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

The determinant of this matrix is $a_{11} a_{22} - a_{12} a_{21}$.

10 Considering a 3 x 3 matrix as shown below:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

The determinant of A can be calculated as:

$$\det. A = a_{11}A_{11} + a_{12}A_{12} + a_{13}A_{13}$$

Where,

15 $A_{11} = (a_{22} a_{33} - a_{23} a_{32})$; $A_{12} = - (a_{21} a_{33} - a_{23} a_{31})$; $A_{13} = (a_{21} a_{32} - a_{22} a_{31})$ are called as cofactors of the elements a_{11} , a_{12} , and a_{13} of matrix A respectively. Along a row or a column, the cofactors will have alternate plus and minus sign with the first cofactor having a positive sign.

The above equation is obtained by using the elements of the first row
20 and the sub matrices obtained by deleting the rows and columns passing through these elements. The same value of determinant can be obtained by

using other rows or any column of the matrix. In general, the determinant of a $n \times n$ square matrix can be written as:

$\det. A = a_{i1}A_{i1} + a_{i2}A_{i2} + \dots + a_{in}A_{in}$ along any row index i , where, $i = 1, 2, \dots, n$

or

5 $\det. A = a_{1j}A_{1j} + a_{2j}A_{2j} + \dots + a_{nj}A_{nj}$ along any column index j , where, $j = 1, 2, \dots, n$

Cofactor

From the above discussion, it is clear that the cofactor of A_{ij} of an element a_{ij} is the factor remaining after the element a_{ij} is factored out. The method of computing the co-factors is explained above for a 3×3 matrix. Along a row or a column the cofactors will have alternate signs of positive and negative with the first cofactor having a positive sign.

Adjoint matrix of a square matrix

The adjoint of a square matrix A is obtained by replacing each element of A with its own cofactor and transposing the result.

Considering a 3×3 matrix as shown below:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

The cofactor matrix containing cofactors (A_{ij} s) of the elements of the above matrix can be written as:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

The adjoint of the matrix A, which is obtained by transposing the cofactor matrix, can be written as:

$$Adj. A = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{bmatrix}$$

Inverse Matrix

- 5 The inverse of matrix A (denoted as A^{-1}) can be obtained by dividing the elements of its adjoint by the determinant.

Singular and Non-Singular Matrices

If the determinant of a square matrix is zero then, it is called a singular matrix. Otherwise, the matrix is known as non-singular.

- 10 The present invention is applied to solve a number of longstanding data analysis problems. These are exemplified as follows.

Multi-collinearity problems

- 15 Multi-collinearity problems arise out of strong correlations. When there are strong correlations, the determinant of correlation matrix tends to become zero thereby making the matrix singular. In such cases, the inverse matrix will be inaccurate or cannot be computed (because determinant term is in the denominator of Equation (2)). As a result, scaled MDs will also be inaccurate or cannot be computed. Such problems can be avoided if we use a matrix form, which is not affected by determinant term. From Equation (2), it is clear that adjoint matrix satisfies this requirement.
- 20

MD values in MTS method are computed by using inverse of the correlation matrix (C^{-1} , where C is correlation matrix). In the present

invention, the adjoint matrix is used to calculate the distances. If MDA denotes the distances obtained from adjoint matrix method, then equation for MDA can be written as:

$$MDA_j = (1/k) Z_{ij} C_{adj} Z_{ij}' \quad (3)$$

- 5 Where, $j = 1 \text{ to } n$
 $Z_{ij} = (z_{1j}, z_{2j}, \dots, z_{kj})$
 = standardized vector obtained by standardized values of X_{ij}
 ($i=1..k$)
 $Z_{ij} = (X_{ij}-m_i)/s_i$;
10 X_{ij} = value of i^{th} characteristic in j^{th} observation
 m_i = mean of i^{th} characteristic
 s_i = s.d. of i^{th} characteristic
 k = number of characteristics/variables
 ' = transpose of the vector
15 C_{adj} = adjoint of the correlation matrix.

The relationship between the conventional MD and the MDAs in Equation (3) can be written as:

$$MD_j = (1/\det.C) MDA_j \quad (4)$$

Thus, an MDA value is similar to a MD value with different properties,
20 that is, the average MDA is not unity. Like in the case of MD values, MDA values represent the distances from the normal group and can be used to measure the degree of abnormalities. In adjoint matrix method also, the Mahalanobis space contains means, standard deviations and correlation structure of the normal or healthy group. Here, the Mahalanobis space cannot
25 be called as unit space since the average of MDAs is not unity.

β -adjustment method

The present invention has applications in multivariate analysis in the presence of small correlation coefficients in correlation matrix. When there are small correlation coefficients, the adjustment factor β is calculated as follows.

$$\begin{aligned} \beta &= 0 \text{ if } r \leq 1/\sqrt{n} \\ \beta &= 1 - \frac{1}{n-1} \left(\frac{1}{r^2} - 1 \right) \text{ if } r > 1/\sqrt{n} \end{aligned} \quad (5)$$

where r is correlation coefficient and n is sample size.

After computing β , the elements of the correlation matrix are adjusted by multiplying them with β . This adjusted matrix is used to carry out MTS analysis or analysis with adjoint matrix.

To explain the applicability of β -adjustment method, Dr. Kanetaka's data on liver disease testing is used. The data contains observations of healthy group as well as of the conditions outside Mahalanobis space (MS). The healthy group (MS) is constructed based on observations on 200 people, who do not have any health problems. There are 17 abnormal conditions. This example is chosen since the correlation matrix in this case contains a few small correlation coefficients. The corresponding β -adjusted correlation matrix (using Equation (5)) is as shown in Table 1.

Table 1: β -adjusted correlation matrix

	X ₁	X ₂	X ₃	X ₄	X ₅	X ₆	X ₇	X ₈	X ₉	X ₁₀	X ₁₁	X ₁₂	X ₁₃	X ₁₄	X ₁₅	X ₁₆	X ₁₇
X ₁	1.000	-0.281	-0.261	-0.392	-0.199	0.052	0.000	0.185	0.277	-0.056	-0.067	0.247	0.099	0.267	-0.276	0.000	-0.265
X ₂	-0.281	1.000	0.055	0.406	0.687	0.271	0.368	-0.061	0.000	0.643	0.384	-0.217	0.252	-0.201	0.885	0.236	0.796
X ₃	-0.261	0.055	1.000	0.417	0.178	0.024	0.103	0.002	0.000	0.149	0.155	0.000	0.127	0.014	0.117	-0.078	0.173
X ₄	-0.392	0.406	0.417	1.000	0.301	0.000	0.000	0.000	-0.059	0.252	0.197	-0.100	0.050	-0.099	0.353	0.036	0.403
X ₅	-0.199	0.687	0.178	0.301	1.000	0.332	0.374	0.000	0.000	0.572	0.419	0.000	0.355	0.000	0.640	0.099	0.671
X ₆	0.052	0.271	0.024	0.000	0.332	1.000	0.788	0.301	0.149	0.544	0.528	0.115	0.305	0.139	0.307	0.154	0.347
X ₇	0.000	0.368	0.103	0.000	0.374	0.788	1.000	0.109	0.000	0.562	0.500	0.097	0.362	0.115	0.387	0.064	0.425
X ₈	0.185	-0.061	0.002	0.000	0.000	0.301	0.109	1.000	0.208	0.090	0.206	0.231	0.054	0.238	0.000	0.043	0.000
X ₉	0.277	0.000	0.000	-0.059	0.000	0.149	0.000	0.208	1.000	0.000	0.113	0.143	0.080	0.139	-0.007	-0.044	0.000
X ₁₀	-0.056	0.643	0.149	0.252	0.572	0.544	0.562	0.090	0.000	1.000	0.679	0.000	0.427	0.016	0.607	0.103	0.645
X ₁₁	-0.067	0.384	0.155	0.197	0.419	0.528	0.500	0.206	0.113	0.679	1.000	0.128	0.329	0.120	0.436	0.000	0.457
X ₁₂	0.247	-0.217	0.000	-0.100	0.000	0.115	0.097	0.231	0.143	0.000	0.128	1.000	0.296	0.966	-0.105	0.000	0.000
X ₁₃	0.099	0.252	0.127	0.050	0.355	0.305	0.362	0.054	0.080	0.427	0.329	0.296	1.000	0.304	0.249	0.000	0.339
X ₁₄	0.267	-0.201	0.014	-0.099	0.000	0.139	0.115	0.238	0.139	0.016	0.120	0.966	0.304	1.000	-0.077	0.000	0.000
X ₁₅	-0.276	0.885	0.117	0.353	0.640	0.307	0.387	0.000	-0.007	0.607	0.436	-0.105	0.249	-0.077	1.000	0.262	0.768
X ₁₆	0.000	0.236	-0.078	0.036	0.099	0.154	0.064	0.043	-0.044	0.103	0.000	0.000	0.000	0.000	0.262	1.000	0.149
X ₁₇	-0.265	0.796	0.173	0.403	0.671	0.347	0.425	0.000	0.000	0.645	0.457	0.000	0.339	0.000	0.768	0.149	1.000

With this matrix, MTS analysis is carried out with dynamic S/N ratio analysis and as a result the following useful variable combination was obtained: X_4 - X_5 - X_7 - X_{10} - X_{12} - X_{13} - X_{14} - X_{15} - X_{16} - X_{17} . This combination is very similar to the useful variable set obtained without β -adjustment; the only
5 difference is presence of variables X_7 and X_{16} .

With this useful variable set, S/N ratio analysis is carried out to measure improvement in overall system performance. From the Table 2, which shows system performance in the form of S/N ratios, it is clear that there is a gain of 0.91 dB units if useful variables are used instead of entire set of
10 variables.

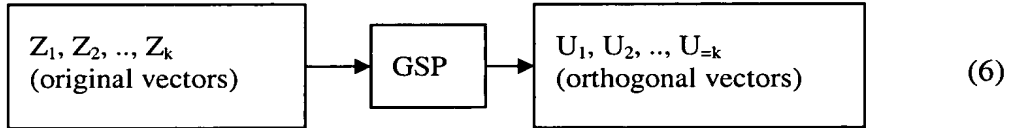
Table 2: S/N Ratio Analysis (β -adjustment method)

S/N ratio-optimal system	43.81 dB
S/N ratio-original system	42.90 dB
Gain	0.91 dB

In an alternate embodiment of the present invention, a Mahalanobis distance is computed using a Gram-Schmidt orthogonalization process (GSP). GSP is often a more robust and sample size insensitive orthogonalization
15 process. Like in MTS, using the inventive MTGS method, the coefficients of orthogonal expansion of unit group are also used to predict the conditions outside this group. The usefulness of this space is tested with signal to noise ratios, like control factors are tested in hardware design. According to the Gram-Schmidt process, original variables are converted to orthogonal and
20 independent variables. The Gram-Schmidt orthogonalization process is

particularly well suited to identify the direction of abnormals. While measuring the degree of abnormality of a given value, a longer distance corresponds to higher degree of severity. In some instances, such as stock performance or financial market predictions, longer distance can represent favorable situations if the normal space is constructed based on companies with average performance. In such an instance, both underperforming and outperforming companies will have longer distances. Distinguishment of these diametrically abnormal situations is preferably performed with the Gram-Schmidt orthogonalization process (GSP).

The GSP operates on a set of given linearly independent vectors Z_1, Z_2, \dots, Z_k , to determine a corresponding set of mutually perpendicular vectors U_1, U_2, \dots, U_k with the same linear span as shown in Equation (6).



The Gram-Schmidt's vectors are constructed sequentially by setting up Equations (7).

$$\begin{aligned}
 U_1 &= Z_1 \\
 U_2 &= Z_2 - ((Z_2' U_1) / (U_1' U_1)) U_1 \\
 &\vdots \\
 U_k &= Z_k - ((Z_k' U_1) / (U_1' U_1)) U_1 - \dots - ((Z_k' U_{k-1}) / (U_{k-1}' U_{k-1})) U_{k-1}
 \end{aligned} \tag{7}$$

Where, ' ' denotes a vector transpose. While calculating MD using GSP, standardized values of the variables are used. Therefore, in the above set of Equations (7), Z_1, Z_2, \dots, Z_k correspond to standardized values.

Calculation of MD Using Gram-Schmidt Process (GSP)

Beginning with a sample of size n , where each sample contains observations on k variables. After standardizing the variables, a set of standardized vectors is obtained. Let these vectors be:

$$\begin{aligned} Z_1 &= (z_{11}, z_{12}, \dots, z_{1n}) \\ Z_2 &= (z_{21}, z_{22}, \dots, z_{2n}) \\ &\vdots \\ Z_k &= (z_{k1}, z_{k2}, \dots, z_{kn}) \end{aligned} \quad (8)$$

After performing GSP, the orthogonal vectors are as follows:

$$\begin{aligned} U_1 &= (u_{11}, u_{12}, \dots, u_{1n}) \\ U_2 &= (u_{21}, u_{22}, \dots, u_{2n}) \\ &\vdots \\ U_k &= (u_{k1}, u_{k2}, \dots, u_{kn}) \end{aligned} \quad (9)$$

It is easily shown that mean of vectors U_1, U_2, \dots, U_k is zero. Let s_1, s_2, \dots, s_k be standard deviations (s.d.s) of U_1, U_2, \dots, U_k respectively. Since the sample of size is n , there are n different MDs. MD corresponding to j^{th} observation of the sample is computed using Equation (10).

$$MD_j = (1/k) [(u_{1j}^2/s_1^2) + (u_{2j}^2/s_2^2) + \dots + (u_{kj}^2/s_k^2)] \quad (10)$$

Where, $j = 1..n$, the values of MD obtained from Equations (1) and (10) are exactly the same. In MTGS methodology, abnormal MDs are computed from the means, standard deviations and Gram-Schmidt coefficients of the normal group or Mahalanobis space, while the Mahalanobis space is a database including means, standard deviations, Gram-Schmidt coefficients and the Mahalanobis distances.

Predictions Based on Gram-Schmidt Variables

According to the present invention, a method of making predictions using Gram-Schmidt (GS) variables without calculating the Mahalanobis distance is provided. This method is useful in situations where the reference group consists of the variables with small or even zero standard deviation or variance. In the most extreme case where if variables have zero standard deviations then correlations with other variables are not possible and hence calculation of Mahalanobis distances is not possible, although variables with zero standard deviations represent very important patterns. This type of situation is frequently seen in pattern recognition problems.

The method of making predictions according to one embodiment of the present invention is described in the following steps:

- 1) Subtract mean vector from all observations in the normal group. Let X_1, X_2, \dots, X_k denote original vectors and L_1, L_2, \dots, L_k denote the vectors that are obtained after subtracting the mean vector.
- 2) Conduct GSP on L_1, L_2, \dots, L_k . If some variables have zero variance or synonymously, zero standard deviation then these variables will be zeroes after subtracting original values from respective means. In such situations these zero vectors also are used as GS vectors because, they will be orthogonal to any other vector. Let U_1, U_2, \dots, U_k denote Gram-Schmidt vectors corresponding to L_1, L_2, \dots, L_k . Here, the reference group consists of means and coefficients of Gram-Schmidt vectors.

3) Obtain Gram-Schmidt vectors corresponding to the observations outside the reference group by using means and Gram-Schmidt coefficients of the reference group.

4) Compute dynamic S/N ratios for Gram-Schmidt variables (U_1, U_2, \dots, U_k)

5 using values of severity of the conditions (observations) as input signals. The severity of conditions can be actual values or optionally, assigned values. The procedure for computing S/N ratios is as follows:

10 If M_1, M_2, \dots, M_t represent the true levels of severity (input signals) corresponding to t abnormals, the relationship between the input signal (M_i s) and the j^{th} variable (U_{ij} s) is given by the following equation:

$$U_{ij} = \beta_j M_i \quad i = 1, \dots, t; j = 1 \dots k \quad \longrightarrow \quad (11)$$

and β_j is the linear slope of relation between U_{ij} and M_i

Then calculate following quantities,

15 $S_T = \text{Total Sum of Squares} = \sum_{i=1}^t U_{ij}^2$

$$r = \text{Sum of squares due to input signal} = \sum_{i=1}^t M_i^2$$

$$S_\beta = \text{Sum of Squares due to Slope} = (1/r) \left[\sum_{i=1}^t M_i U_{ij} \right]^2$$

$$S_e = \text{Error Sum of Squares} = S_T - S_\beta$$

$$V_e = \text{Error Variance} = S_e / (t-1)$$

20 The linear slope, β_j , for j^{th} variable is given by:

$$\beta_j = [\sum_{i=1}^t M_i U_{ij}] / r \quad (12)$$

The S/N ratio, η_j , corresponding j^{th} variable is given by,

$$\eta_j = \beta_j^2 / V_e \quad (13)$$

- 5 5) After computing η_j and β_j for each Gram-Schmidt variable calculate predicted values of abnormals. The predicted value of i^{th} abnormal condition is obtained as follows:

$$Y_i = \frac{\sum_{j=1}^k \left(\frac{\eta_j U_{ij}}{\beta_j} \right)}{\sum_{j=1}^k \eta_j} \quad (14)$$

where, $i=1,...,t$ and U_{ij} is Gram-Schmidt element corresponding to j^{th} variable in i^{th} condition.

- 10 6) If there is a good correlation between the predicted values and actual values then Equation (14) is useful for future predictions. Again here, we can use S/N ratio to examine the accuracy of the prediction, that is, the correlation between predicted values and actual values.

Multiple Mahalanobis distance

- 15 Selection of suitable subsets is very important in multivariate diagnosis/pattern recognition activities as it is difficult to handle large datasets with several numbers of variables. The present invention applies a new metric called Multiple Mahalanobis Distance (MMD) for computing S/N ratios to select suitable subsets. This method is useful in complex situations, illustratively including voice recognition or TV picture recognition. In these
- 20

cases, the number of variables runs into the order of several thousands. Use of MMD method helps in reducing the problem complexity and to make effective decisions in complex situations.

5 In MMD method, large number of variables is divided into several subsets containing local variables. For example, in a voice recognition pattern (as shown in Figure 2), let there be k subsets. The subsets correspond to k patterns numbered from 1,2,... k . Each pattern starts at a low value, reaches a maximum and then again returns to the low value. These patterns (subsets) are described by a set of respective local variables. In MMD method, for each
10 subset the Mahalanobis distances are calculated. These Mahalanobis distances are used to calculate MMD. Using abnormal MMDs, S/N ratios are calculated to determine useful subsets. In this way the complexity of the problems is reduced.

This method is also useful for identifying the subsets (or variables in
15 the subsets) corresponding to different failure modes or patterns that are responsible for higher values of MDs. For example in the case of final product inspection system, use of MMD method would help to find out variables corresponding to different processes that are responsible for product failure.

If the variables corresponding to different subsets or processes cannot
20 be identified then, decision-maker can select subsets from the original set of variables and identify the best subsets required.

Exemplary Steps in Inventive Process

1. Define subsets from original set of variables. The subsets may contain variables corresponding to different patterns or failure modes. These variables can also be based on decision maker's discretion. The number of variables in the subsets need not be the same.
2. For each subset, calculate MDs (for normals and abnormals) using respective variables in them.
3. Compute square root of these MDs ($\sqrt{\text{MDs}}$).
4. Consider the subsets as variables (control factors). The $\sqrt{\text{MDs}}$ would provide required data for these subsets. If there are k subsets then, the problem is similar to MTS problem with k variables. The number of normals and abnormals will be same as in the original problem. The analysis with $\sqrt{\text{MDs}}$ is exactly similar to that of MTS method with original variables. The new Mahalanobis distance obtained based on square root of MDs is referred to as Multiple Mahalanobis Distance (MMD).
5. With the MMDs, S/N ratios are obtained for each run of an orthogonal array. Based on gains in S/N ratios, the important subsets are selected.

Example 1

The adjoint matrix method is applied to liver disease test data considered earlier. For the purpose of better understanding of the discussion, correlation matrix, inverse matrix and adjoint matrix corresponding to the 17

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variables are given in Tables 3, 4, and 5 respectively. In this case the determinant of the correlation matrix is 0.00001314.

5 The Mahalanobis distances calculated by inverse matrix method and adjoint matrix method (MDAs), are given in Table 6 (for normal group) and in Table 7 (for abnormal group). From the Table 6, it is clear that the average MDAs for normals do not converge to 1.0. MDAs and MDs are related according to the Equation (4).

Table 3: Correlation matrix

	X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17
X1	1.000	-0.297	-0.278	-0.403	-0.220	0.101	0.041	0.208	0.293	-0.104	-0.112	0.264	0.135	0.283	-0.292	-0.019	-0.282
X2	-0.297	1.000	0.103	0.416	0.690	0.287	0.379	-0.108	-0.048	0.647	0.395	-0.237	0.269	-0.222	0.886	0.254	0.798
X3	-0.278	0.103	1.000	0.427	0.202	0.084	0.139	0.072	0.011	0.177	0.182	0.070	0.158	0.078	0.150	-0.119	0.198
X4	-0.403	0.416	0.427	1.000	0.315	0.038	0.056	0.010	-0.106	0.269	0.219	-0.136	0.100	-0.135	0.365	0.091	0.413
X5	-0.220	0.690	0.202	0.315	1.000	0.345	0.385	0.063	-0.057	0.578	0.429	0.012	0.367	0.032	0.644	0.135	0.675
X6	0.101	0.287	0.084	0.038	0.345	1.000	0.790	0.316	0.177	0.550	0.535	0.148	0.320	0.168	0.321	0.181	0.359
X7	0.041	0.379	0.139	0.056	0.385	0.790	1.000	0.143	0.068	0.568	0.507	0.134	0.373	0.148	0.398	0.109	0.435
X8	0.208	-0.108	0.072	0.010	0.063	0.316	0.143	1.000	0.229	0.129	0.227	0.250	0.103	0.257	-0.063	0.095	-0.015
X9	0.293	-0.048	0.011	-0.106	-0.057	0.177	0.068	0.229	1.000	0.065	0.147	0.171	0.121	0.168	-0.075	-0.096	-0.061
X10	-0.104	0.647	0.177	0.269	0.578	0.550	0.568	0.129	0.065	1.000	0.683	0.052	0.437	0.079	0.612	0.138	0.649
X11	-0.112	0.395	0.182	0.219	0.429	0.535	0.507	0.227	0.147	0.683	1.000	0.159	0.342	0.152	0.445	0.048	0.465
X12	0.264	-0.237	0.070	-0.136	0.012	0.148	0.134	0.250	0.171	0.052	0.159	1.000	0.310	0.967	-0.140	-0.004	-0.023
X13	0.135	0.269	0.158	0.100	0.367	0.320	0.373	0.103	0.121	0.437	0.342	0.310	1.000	0.318	0.267	-0.041	0.352
X14	0.283	-0.222	0.078	-0.135	0.032	0.168	0.148	0.257	0.168	0.079	0.152	0.967	0.318	1.000	-0.119	0.025	-0.011
X15	-0.292	0.886	0.150	0.365	0.644	0.321	0.398	-0.063	-0.075	0.612	0.445	-0.140	0.267	-0.119	1.000	0.279	0.771
X16	-0.019	0.254	-0.119	0.091	0.135	0.181	0.109	0.095	-0.096	0.138	0.048	-0.004	-0.041	0.025	0.279	1.000	0.177
X17	-0.282	0.798	0.198	0.413	0.675	0.359	0.435	-0.015	-0.061	0.649	0.465	-0.023	0.352	-0.011	0.771	0.177	1.000

Table 4: Inverse matrix

	X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17
X1	1.592	-0.003	0.307	0.297	0.118	-0.082	-0.116	-0.193	-0.304	-0.113	0.248	0.337	-0.284	-0.552	0.146	-0.028	0.198
X2	-0.003	8.136	0.658	-0.706	-1.281	0.627	-0.439	0.379	-0.576	-1.482	0.748	-0.192	-0.077	1.358	-4.277	-0.316	-1.525
X3	0.307	0.658	1.442	-0.594	-0.169	0.136	-0.258	-0.066	-0.123	-0.115	0.070	0.223	-0.097	-0.304	-0.315	0.194	-0.023
X4	0.297	-0.706	-0.594	1.677	0.101	0.009	0.272	-0.143	0.088	0.071	-0.157	0.026	-0.049	0.055	0.317	-0.103	-0.296
X5	0.118	-1.281	-0.169	0.101	2.357	-0.197	0.110	-0.193	0.200	-0.034	-0.121	0.210	-0.235	-0.440	0.077	0.108	-0.429
X6	-0.082	0.627	0.136	0.009	-0.197	3.403	-2.266	-0.483	-0.297	-0.436	-0.348	0.332	0.044	-0.156	-0.108	-0.338	-0.104
X7	-0.116	-0.439	-0.258	0.272	0.110	-2.266	3.192	0.275	0.252	-0.172	-0.133	-0.240	-0.195	0.106	-0.009	0.147	-0.153
X8	-0.193	0.379	-0.066	-0.143	-0.193	-0.483	0.275	1.338	-0.157	-0.056	-0.179	-0.103	0.064	-0.028	0.022	-0.143	0.012
X9	-0.304	-0.576	-0.123	0.088	0.200	-0.297	0.252	-0.157	1.247	0.101	-0.218	-0.118	-0.034	-0.006	0.240	0.157	0.131
X10	-0.113	-1.482	-0.115	0.071	-0.034	-0.436	-0.172	-0.056	0.101	3.321	-1.247	0.928	-0.335	-1.004	0.386	0.041	-0.350
X11	0.248	0.748	0.070	-0.157	-0.121	-0.348	-0.133	-0.179	-0.218	-1.247	2.302	-0.880	-0.001	0.754	-0.637	0.151	-0.036
X12	0.337	-0.192	0.223	0.026	0.210	0.332	-0.240	-0.103	-0.118	0.928	-0.880	16.234	-0.293	-15.614	0.589	0.274	-0.363
X13	-0.284	-0.077	-0.097	-0.049	-0.235	0.044	-0.195	0.064	-0.034	-0.335	-0.001	-0.293	1.537	-0.096	0.043	0.167	-0.145
X14	-0.552	1.358	-0.304	0.055	-0.440	-0.156	0.106	-0.028	-0.006	-1.004	0.754	-15.614	-0.096	16.526	-0.826	-0.463	-0.018
X15	0.146	-4.277	-0.315	0.317	0.077	-0.108	-0.009	0.022	0.240	0.386	-0.637	0.589	0.043	-0.826	5.415	-0.330	-0.691
X16	-0.028	-0.316	0.194	-0.103	0.108	-0.338	0.147	-0.143	0.157	0.041	0.151	0.274	0.167	-0.463	-0.330	1.249	0.120
X17	0.198	-1.525	-0.023	-0.296	-0.429	-0.104	-0.153	0.012	0.131	-0.350	-0.036	-0.363	-0.145	-0.018	-0.691	0.120	3.599

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Table 5: Adjoint matrix

	X ₁	X ₂	X ₃	X ₄	X ₅	X ₆	X ₇	X ₈	X ₉	X ₁₀	X ₁₁	X ₁₂	X ₁₃	X ₁₄	X ₁₅	X ₁₆	X ₁₇
X ₁	2.09E-05	-3.8E-08	4.03E-06	3.9E-06	1.55E-06	-1.07E-06	-1.52E-06	-2.53E-06	-4E-06	-1.49E-06	3.26E-06	4.43E-06	-3.73E-06	-7.25E-06	1.92E-06	-3.63E-07	2.6E-06
X ₂	-3.8E-08	0.000107	8.65E-06	-9.27E-06	-1.68E-05	8.24E-06	-5.77E-06	4.98E-06	-7.57E-06	-1.95E-05	9.83E-06	-2.53E-06	-1.01E-06	1.78E-05	-5.62E-05	4.16E-06	-2E-05
X ₃	4.03E-06	8.65E-06	1.89E-05	-7.81E-06	-2.22E-06	1.78E-06	-3.4E-06	-8.65E-07	-1.62E-06	-1.51E-06	9.22E-07	2.93E-06	-1.27E-06	-3.99E-06	4.13E-06	2.55E-06	-3.04E-07
X ₄	3.9E-06	-9.27E-06	-7.81E-06	2.2E-05	1.33E-06	1.18E-07	3.57E-06	-1.88E-06	1.16E-06	9.35E-07	-2.06E-06	3.41E-07	-6.46E-07	7.2E-07	4.17E-06	-1.36E-06	-3.89E-06
X ₅	1.55E-06	-1.68E-05	-2.22E-06	1.33E-06	3.1E-05	-2.59E-06	1.44E-06	-2.54E-06	2.63E-06	-4.5E-07	-1.6E-06	2.77E-06	-3.09E-06	-5.78E-06	1.02E-06	1.42E-06	-5.64E-06
X ₆	-1.07E-06	8.24E-06	1.78E-06	1.18E-07	-2.59E-06	4.47E-05	-2.98E-05	-6.35E-06	-3.91E-06	-5.74E-06	-4.57E-06	4.36E-06	5.75E-07	-2.05E-06	-1.42E-06	-4.44E-06	-1.37E-06
X ₇	-1.52E-06	-5.77E-06	-3.4E-06	3.57E-06	1.44E-06	-2.98E-05	4.19E-05	3.61E-06	3.31E-06	-2.26E-06	-1.75E-06	-3.16E-06	-2.56E-06	1.4E-06	-1.18E-07	1.94E-06	-2.01E-06
X ₈	-2.53E-06	4.98E-06	-8.65E-07	-1.88E-06	-2.54E-06	6.35E-06	3.61E-06	1.76E-05	-2.07E-06	-7.31E-07	-2.35E-06	-1.35E-06	8.37E-07	-3.73E-07	2.92E-07	-1.87E-06	1.61E-07
X ₉	-4E-06	-7.57E-06	-1.62E-06	1.16E-06	2.63E-06	-3.91E-06	3.31E-06	-2.07E-06	1.64E-05	1.32E-06	-2.86E-06	-1.56E-06	-4.48E-07	-8.37E-08	3.15E-06	2.06E-06	1.72E-06
X ₁₀	-1.49E-06	-1.95E-05	-1.51E-06	9.35E-07	-4.5E-07	-5.74E-06	-2.26E-06	-7.31E-07	1.32E-06	4.36E-05	-1.64E-05	1.22E-05	-4.41E-06	-1.32E-05	5.07E-06	5.42E-07	-4.59E-06
X ₁₁	3.26E-06	9.83E-06	9.22E-07	-2.06E-06	-1.6E-06	-4.57E-06	-1.75E-06	-2.35E-06	-2.86E-06	-1.64E-05	3.02E-05	-1.16E-05	-1.73E-08	9.91E-06	-8.37E-06	1.98E-06	-4.68E-07
X ₁₂	4.43E-06	-2.53E-06	2.93E-06	3.41E-07	2.77E-06	4.36E-06	-3.16E-06	-1.35E-06	-1.56E-06	1.22E-05	-1.16E-05	0.000213	-3.85E-06	-0.000205	7.74E-06	3.6E-06	-4.77E-06
X ₁₃	-3.73E-06	-1.01E-06	-1.27E-06	-6.46E-07	-3.09E-06	5.75E-07	-2.56E-06	8.37E-07	-4.48E-07	1.22E-05	-1.73E-08	-3.85E-06	2.02E-05	-1.27E-06	5.62E-07	2.19E-06	-1.9E-06
X ₁₄	-7.25E-06	1.78E-05	-3.99E-06	7.2E-07	-5.78E-06	-2.05E-06	1.4E-06	-3.73E-07	-8.37E-08	-1.32E-05	9.91E-06	-0.000205	-1.27E-06	0.000217	-1.09E-05	-6.08E-06	-2.41E-07
X ₁₅	1.92E-06	-5.62E-05	-4.13E-06	4.17E-06	1.02E-06	-1.42E-06	-1.18E-07	2.92E-07	3.15E-06	5.07E-06	-8.37E-06	7.74E-06	5.62E-07	-1.09E-05	7.12E-05	-4.34E-06	-9.08E-06
X ₁₆	-3.63E-07	-4.16E-06	2.55E-06	-1.36E-06	1.42E-06	-4.44E-06	1.94E-06	-1.87E-06	2.06E-06	5.42E-07	1.98E-06	3.6E-06	2.19E-06	-6.08E-06	-4.34E-06	1.64E-05	1.58E-06
X ₁₇	2.6E-06	-2E-05	-3.04E-07	-3.89E-06	-5.64E-06	-1.37E-06	-2.01E-06	1.61E-07	1.72E-06	-4.59E-06	-4.68E-07	-4.77E-06	-1.9E-06	-2.41E-07	-9.08E-06	1.58E-06	4.73E-05

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Table 6: MDs and MDAs for normal group

S.No.	1	2	3	4	5	6	7	8	...	196	197	198	199	200	Average
MD-inverse	0.378374	0.431373	0.403562	0.500211	0.515396	0.495501	0.583142	0.565654	...	1.74	1.75	1.78	1.76	2.36	0.995
MD-Adj int	0.000005	0.000006	0.000005	0.000007	0.000007	0.000007	0.000008	0.000007	...	0.00002	0.00002	0.00002	0.00002	0.00003	0.000013

Table 7: MDs and MDAs for abnormal

S.No	1	2	3	4	5	6	7	8	...	13	14	15	16	17	Av rage
MD-Inv rs	7.72741	8.41629	10.29148	7.20516	10.59075	10.55711	13.31775	14.81278	...	19.65543	43.04050	78.64045	97.27242	135.70578	30.39451
MD-adjoint	0.00010	0.00011	0.00014	0.00009	0.00014	0.00014	0.00017	0.00019	...	0.00026	0.00057	0.00103	0.00128	0.00178	0.00040

$L_{32}(2^{31})$ OA is used to accommodate 17 variables. Table 8 gives dynamic S/N ratios for all the combinations of this array with inverse matrix method and adjoint matrix method. Table 9 shows gain in S/N ratios for both the methods. It is clear that gains in S/N ratios are same for both methods.

5 The important variable combination based on these gains is: X_4 - X_5 - X_{10} - X_{12} - X_{13} - X_{14} - X_{15} - X_{17} . From Table 10, which shows system performance in the form of S/N ratios, it is clear that there is a gain of 1.98 dB units if useful variables are used instead of all the variables. This gain is also exactly same as that obtained in inverse matrix method.

10 Hence, even if an adjoint matrix method is used, the ultimate results would be the same. However, MDA values are advantageous because it will not take into account the determinant of correlation matrix. In case of multicollinearity problems, as the determinant tend to become zero, the inverse matrix becomes inefficient giving rise to inaccurate MDs. Such problems can
15 be avoided if MDAs are used based on adjoint matrix method.

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Table 8: Dynamic S/N ratios for the combinations of $L_{32}(2^{31})$ array

Run	S/N ratio (Inverse)	S/N ratio (Adjoint)
1	-6.252	42.560
2	-6.119	42.693
3	-10.024	38.788
4	-10.181	38.631
5	-10.348	38.464
6	-10.495	38.317
7	-7.934	40.878
8	-8.177	40.635
9	-9.234	39.578
10	-9.631	39.181
11	-3.338	45.474
12	-3.406	45.406
13	-10.932	37.880
14	-11.121	37.691
15	-6.495	42.317
16	-7.265	41.547
17	-7.898	40.914
18	-7.665	41.147
19	-10.156	38.656
20	-9.901	38.911
21	-5.431	43.381
22	-5.312	43.500
23	-7.603	41.209
24	-7.498	41.314
25	-11.412	37.400
26	-11.100	37.712
27	-5.874	42.938
28	-4.989	43.823
29	-9.238	39.574
30	-8.989	39.823
31	-5.544	43.268
32	-5.303	43.509

Table 9: Gain in S/N Ratios

Inverse Method				Adjoint Method			
Variable	Level 1	Level 2	Gain	Variable	Level 1	Level 2	Gain
X ₁	-8.185	-7.745	-0.440	X ₁	40.627	41.067	-0.440
X ₂	-8.187	-7.742	-0.445	X ₂	40.625	41.070	-0.445
X ₃	-8.249	-7.680	-0.569	X ₃	40.563	41.132	-0.569
X ₄	-7.949	-7.980	0.031	X ₄	40.863	40.832	0.031
X ₅	-7.069	-8.860	1.791	X ₅	41.743	39.952	1.791
X ₆	-8.318	-7.611	-0.706	X ₆	40.494	41.201	-0.706
X ₇	-7.976	-7.954	-0.022	X ₇	40.836	40.858	-0.022
X ₈	-8.824	-7.105	-1.718	X ₈	39.988	41.707	-1.718
X ₉	-8.188	-7.742	-0.446	X ₉	40.625	41.070	-0.446
X ₁₀	-6.358	-9.571	3.212	X ₁₀	42.454	39.241	3.212
X ₁₁	-8.101	-7.828	-0.273	X ₁₁	40.711	40.984	-0.273
X ₁₂	-7.821	-8.108	0.287	X ₁₂	40.991	40.704	0.287
X ₁₃	-7.562	-8.367	0.805	X ₁₃	41.250	40.445	0.805
X ₁₄	-7.315	-8.615	1.300	X ₁₄	41.497	40.197	1.300
X ₁₅	-7.590	-8.339	0.749	X ₁₅	41.222	40.473	0.749
X ₁₆	-7.982	-7.947	-0.035	X ₁₆	40.830	40.865	-0.035
X ₁₇	-7.832	-8.097	0.265	X ₁₇	40.980	40.715	0.265

Table 10: S/N Ratio Analysis

S/N ratio-optimal system	44.54 dB
S/N ratio-original system	42.56 dB
Gain	1.98 dB

Example 2

5 The adjoint matrix method is applied to another case with 12 variables. In this example, there are 58 normals and 30 abnormals. The MDs corresponding to normals are computed by using MTS method – the average MD is 0.92. The reason for this discrepancy is the existence of multi-collinearity. This is clear from the correlation matrix (Table 11), which shows

10 that the variables X₁₀, X₁₁ and X₁₂ have high correlations with each other. The

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determinant of the matrix is also estimated and it is found to be 8.693×10^{-12} (close to zero), indicating that the matrix is almost singular. Presence of multicollinearity will also affect the other stages of the MTS method. Hence, adjoint matrix method is used to perform the analysis.

5 **Adjoint Matrix Method**

The adjoint of correlation matrix is shown in Table 12.

Table 11: Correlation Matrix

	X ₁	X ₂	X ₃	X ₄	X ₅	X ₆	X ₇	X ₈	X ₉	X ₁₀	X ₁₁	X ₁₂
X ₁	1	0.358	-0.085	-0.024	0.005	0.057	-0.149	-0.128	-0.046	0.105	-0.055	-0.055
X ₂	0.358	1	0.014	0.022	0.003	-0.097	-0.271	-0.079	0.061	0.325	0.023	0.023
X ₃	-0.085	0.014	1	0.0769	0.0708	0.0577	0.3138	0.1603	0.0815	0.4945	0.5286	0.5333
X ₄	-0.024	0.022	0.0769	1	-0.135	-0.018	0.296	-0.206	0.062	0.597	0.624	0.622
X ₅	0.005	0.003	0.0708	-0.135	1	0.123	0.264	0.114	0.053	0.536	0.560	0.559
X ₆	0.057	-0.097	0.0577	-0.018	0.123	1	0.353	0.055	0.056	0.063	0.096	0.096
X ₇	-0.149	-0.271	0.3138	0.296	0.264	0.353	1	0.103	0.092	0.395	0.508	0.508
X ₈	-0.128	-0.079	0.1603	-0.206	0.114	0.055	0.103	1	-0.153	-0.032	-0.002	-0.0004
X ₉	-0.046	0.061	0.0815	0.062	0.053	0.056	0.092	-0.153	1	0.116	0.104	0.104
X ₁₀	0.105	0.325	0.4945	0.597	0.536	0.063	0.395	-0.032	0.116	1	0.951	0.951
X ₁₁	-0.055	0.023	0.5286	0.624	0.560	0.096	0.508	-0.002	0.104	0.951	1	0.999
X ₁₂	-0.055	0.023	0.5333	0.622	0.559	0.096	0.508	-0.0004	0.104	0.951	0.999	1

Table 12: Adjoint Matrix

	X ₁	X ₂	X ₃	X ₄	X ₅	X ₆	X ₇	X ₈	X ₉	X ₁₀	X ₁₁	X ₁₂
X ₁	1.00912E-10	4.70272E-10	1.61623E-10	2.76032E-10	2.57713E-10	-5.48951E-12	5.043E-12	7.14809E-13	1.43647E-12	-1.66567E-09	7.66095E-10	4.08691E-10
X ₂	4.70263E-10	2.50034E-09	9.18237E-10	1.55621E-09	1.45406E-09	-2.10511E-11	2.83118E-11	-3.03613E-12	8.03373E-13	-8.7444E-09	4.41674E-09	1.58527E-09
X ₃	1.61527E-10	9.17746E-10	1.06463E-09	1.63137E-09	1.50922E-09	5.28862E-13	2.04944E-11	-9.18812E-12	-1.3292E-11	-3.18575E-09	5.69418E-09	-5.10159E-09
X ₄	2.7594E-10	1.55576E-09	1.63154E-09	2.56985E-09	2.37158E-09	-3.57245E-13	3.50392E-11	-1.10855E-11	-1.89581E-11	-5.40857E-09	6.24469E-09	-4.93127E-09
X ₅	2.57631E-10	1.45366E-09	1.50339E-09	2.37159E-09	2.20389E-09	-1.73783E-12	3.34823E-11	-1.29848E-11	-1.78615E-11	-5.0537E-09	5.64554E-09	-4.38529E-09
X ₆	-5.4903E-12	-2.10556E-11	5.23064E-13	-3.64155E-13	-1.74411E-12	1.06058E-11	-4.37752E-12	-1.97695E-13	-5.79622E-13	7.5335E-11	3.17881E-13	-6.9595E-11
X ₇	5.04604E-12	2.83284E-11	2.05079E-11	3.50574E-11	3.34989E-11	-4.37759E-12	1.58563E-11	-1.42556E-12	-1.00253E-12	-8.62928E-11	-1.25906E-10	1.486E-10
X ₈	7.12086E-13	-3.11071E-12	-9.19606E-12	-1.10978E-11	-1.29962E-11	-1.97598E-13	-1.42569E-12	1.01743E-11	1.84668E-12	1.04492E-11	1.34899E-10	-1.25096E-10
X ₉	1.43722E-12	8.07304E-13	-1.32908E-11	-1.89556E-11	-1.78591E-11	-5.79657E-13	-1.00246E-12	1.84666E-12	9.48854E-12	-6.93471E-12	-2.47767E-11	5.98708E-11
X ₁₀	-1.66565E-09	-8.74446E-09	-3.1875E-09	-5.4102E-09	-5.05514E-09	7.53194E-11	-8.62349E-11	1.03982E-11	-6.92086E-12	3.07209E-08	-1.50768E-08	-6.10343E-09
X ₁₁	7.60305E-10	4.38609E-09	5.67096E-09	6.22205E-09	5.62443E-09	5.56545E-13	-1.26234E-10	1.35001E-10	-2.47494E-11	-1.49692E-08	2.88114E-07	-2.83899E-07
X ₁₂	4.14615E-10	1.61673E-09	-5.08692E-09	-4.90701E-09	-4.36272E-09	-6.98238E-11	1.48962E-10	-1.25168E-10	5.98339E-11	-6.21375E-09	-2.8383E-07	2.97854E-07

After computing MDA values for normals, the measurement scale is validated by computing abnormal MDA values. Figure 3 indicates that there is a clear distinction between normals and abnormals.

In the next step, important variables are selected using $L_{16}(2^{15})$ array.

- 5 The S/N ratio analysis was performed based on larger-the-better criterion in usual way. The gains in S/N ratios are shown in Table 13. From this table, it is clear that the variables X_1 - X_2 - X_3 - X_4 - X_6 - X_{10} - X_{11} - X_{12} have positive gains and hence they are important. The confirmation run with these variables (Figure 4) indicates that distinction (between normals and abnormals) is very
- 10 good.

Table 13: Gain in S/N ratio

Variable	Level 1	Level 2	Gain
X_1	-102.90	-105.01	2.12
X_2	-103.53	-104.38	0.86
X_3	-103.84	-104.07	0.22
X_4	-103.72	-104.19	0.47
X_5	-104.04	-103.86	-0.18
X_6	-103.87	-104.04	0.16
X_7	-104.18	-103.72	-0.46
X_8	-104.14	-103.77	-0.37
X_9	-104.33	-103.58	-0.76
X_{10}	-103.51	-104.40	0.90
X_{11}	-103.78	-104.13	0.35
X_{12}	-103.43	-104.48	1.05

Therefore, adjoint matrix method can safely replace inverse matrix method as it is as efficient as inverse matrix method in general and more efficient when there are problems of multi-collinearity.

Example 3

From the 17 variables, eight subsets (as shown in Table 14) are selected. These subsets are selected to illustrate the MMD methodology; there is no rational for this selection. It is to be noted that the number of variables in each subset are not the same.

Table 14: Subsets for MMD analysis

Subset	Variables
S ₁	X ₁ -X ₂ -X ₃ -X ₄
S ₂	X ₅ -X ₆ -X ₇ -X ₈
S ₃	X ₉ -X ₁₀ -X ₁₁ -X ₁₂
S ₄	X ₁₃ -X ₁₄ -X ₁₅ -X ₁₆ -X ₁₇
S ₅	X ₃ -X ₄ -X ₅ -X ₆
S ₆	X ₁₀ -X ₁₁ -X ₁₂ -X ₁₃ -X ₁₄ -X ₁₅
S ₇	X ₁₄ -X ₁₅ -X ₁₆ -X ₁₇
S ₈	X ₂ -X ₅ -X ₇ -X ₁₀ -X ₁₂ -X ₁₃ -X ₁₄ -X ₁₅

For each subset, Mahalanobis distances are computed with the help of correlation matrices of respective variables. Therefore, we have eight sets of MDs (for normals and abnormals) corresponding to the subsets. The $\sqrt{\text{MDs}}$ provide data corresponding to the subsets that are considered as control factors. Tables 15 and 16 show sample data ($\sqrt{\text{MDs}}$) for normals and abnormals.

Table 15: $\sqrt{\text{MDs}}$ for normals (sample data)

S.No	S ₁	S ₂	S ₃	S ₄	S ₅	S ₆	S ₇	S ₈
1	0.873	0.545	0.707	0.756	0.796	0.505	0.832	0.574
2	0.762	0.540	0.929	0.710	0.499	0.688	0.606	0.807
3	1.022	0.688	0.550	0.623	0.955	0.479	0.697	0.613
4	1.102	0.544	0.769	0.740	1.225	0.648	0.827	0.681
5	1.022	0.640	0.602	0.888	0.815	0.782	0.934	0.695
....
196	1.041	0.786	1.691	1.513	0.500	1.550	1.539	1.411
197	1.467	1.310	2.101	1.201	1.457	1.481	0.611	1.373
198	1.086	1.278	0.974	1.406	1.410	1.834	0.994	1.648
199	1.238	0.999	1.107	1.061	1.206	1.132	0.964	1.700
200	1.391	0.924	0.979	0.680	1.094	2.156	0.750	1.844

Table 16: $\sqrt{\text{MDs}}$ for abnormals (sample data)

S.No	S ₁	S ₂	S ₃	S ₄	S ₅	S ₆	S ₇	S ₈
1	1.339	2.930	2.610	3.428	2.574	3.277	2.913	3.734
2	1.491	3.469	1.931	1.511	3.267	3.388	1.687	3.932
3	1.251	2.700	0.742	2.631	2.447	3.322	2.660	4.365
4	2.124	2.507	2.041	3.240	2.518	3.058	2.009	3.395
5	1.010	2.182	2.867	1.279	1.861	4.035	1.090	4.440
....
13	1.769	2.819	6.544	2.153	2.352	6.023	2.177	5.776
14	1.898	2.045	3.817	4.551	2.443	10.213	1.969	9.275
15	1.624	12.681	2.116	3.672	12.248	9.064	1.202	11.426
16	5.453	13.314	3.630	1.022	13.515	10.095	1.108	12.121
17	4.511	16.425	5.489	3.684	12.027	11.142	2.264	10.939

After arranging the data ($\sqrt{\text{MDs}}$) in this manner, MMD analysis is carried out. In this analysis, MMDs are Mahalanobis distances obtained from $\sqrt{\text{MDs}}$. Table 17 and 18 provide sample values of MMDs for normals and abnormals respectively.

Table 17: MMDs for normals (sample values)

Condition	1	2	3	4	5	6	7	8	9	10	...	198	199	200
MMD	0.558	0.861	0.425	0.786	0.413	1.655	0.357	0.660	0.641	0.717	...	2.243	2.243	4.979

Table 18: MMDs for abnormals (sample values)

Condition	1	2	3	4	5	6	7	8	9	10	...	15	16	17
MMD	22.52	29.86	30.61	23.47	27.05	57.12	61.61	52.64	50.77	66.15	...	515.50	601.30	592.37

The next step is to assign the subsets to the columns of a suitable orthogonal array. Since there are eight subsets, $L_{12}(2^{11})$ array was selected. The abnormal MMDs are computed for each run of this array. After performing average response analysis, gains in S/N ratios are computed for all the subsets. These details are shown in Table 19.

Table 19: Gain in S/N ratios

	Level 1	Level 2	Gain
S₁	15.498	18.053	-2.555
S₂	17.463	16.089	1.374
S₃	16.712	16.839	-0.127
S₄	15.925	17.627	-1.702
S₅	17.626	15.926	1.700
S₆	17.243	16.309	0.934
S₇	15.683	17.869	-2.186
S₈	18.556	14.996	3.560

From this table it is clear that S_8 has highest gain indicating that this is very important subset. It should be noted that the variables in this subset are same as the useful variables obtained from MTS method. This example is a simple case where we have only 17 variables and therefore here, MMD method may not be necessary. However, in complex cases, with several hundreds of variables, MMD method is more appropriate and reliable.

Example 4

In order to demonstrate the applicability of Gram-Schmidt process to predict abnormal conditions without computing the Mahalanobis distances, it is applied to the medical diagnosis case example previously discussed with 17

abnormal conditions. Out of 17 conditions, the first ten conditions are considered mild and the remaining seven conditions are considered as medium. This judgment was made by Dr. Kanetaka, who is a liver disease diagnosis specialist in Japan. For the purposes of prediction and since true values of severity are unknown, a value of 3 is assigned for the mild group and a value of 9 is assigned for the medium group. Table 20 provides the summary of data analysis for abnormals in this case example generated by GSP. Figure 5 shows that there is a good match between actual level of severity and predicted values.

Intentionally, two variables with zero standard deviations are introduced. These variables are considered as the first and second variables and now the total number of variables is 19. Table 21 provides the summary of data analysis for abnormals in this instance. Like the data of Figure 5, there is a good match between actual level of severity and predicted values as shown in Figure 6.

Table 20: Summary of data analysis

Abnormal	Mi(°)	U1	U2	U3	U4	U5	U6	U7	U8	U9	U10	U11	U12	U13	U14	U15	U16	U17	Yi (Predicted)
13		12.3150	-4.3293	0.5390	-0.1329	-275.8953	8.9867	3.6369	39.6987	3.9237	-4.9805	-6.0171	91.7303	185.2230	10.9136	0.3937	2.6036	-0.0004	3.2929
23		16.3150	-3.8353	-0.5307	-0.1940	-319.9262	18.5124	10.4489	8.8425	121.4416	38.7007	3.1131	15.1255	22.6190	40.5201	-0.1010	-1.7837	0.1866	4.1392
33		7.3150	-4.9467	-0.4990	-0.1476	-290.7776	5.0656	-2.3387	37.3756	14.1496	13.9428	1.1665	15.5386	146.1268	34.6194	0.9444	-2.8997	0.3113	3.2915
43		8.3150	4.1768	0.8948	-0.3463	-290.5790	7.1602	6.2609	33.9778	-6.3051	9.1650	-16.1595	59.3059	190.3586	11.0576	-0.0293	-0.5074	-1.1519	4.3706
53		7.3150	4.0533	0.1872	-0.2073	-343.8372	-1.7947	2.2598	-13.7225	107.8699	100.2455	-3.5307	-9.7133	59.8334	41.1504	-0.1751	-2.4316	0.3238	3.9720
63		6.3150	3.9298	-0.0204	0.0298	-291.4935	22.5440	42.6023	25.0359	46.8510	-26.2873	-11.2102	56.9628	12.4162	22.8997	0.1299	-3.6248	0.2957	3.8183
73		6.3150	3.9298	-0.0204	0.0298	-291.4935	22.5440	42.6023	25.0359	46.8510	-26.2873	-11.2102	56.9628	12.4162	40.6997	0.0817	-4.4633	0.2882	4.0515
83		15.3150	5.0412	0.0479	-0.2370	-341.6418	2.4900	10.2859	24.1717	-39.7420	11.8856	-2.4939	73.6173	306.5702	40.4239	-0.0696	1.4407	0.3877	5.5233
93		10.3150	4.4238	-0.3900	-0.0740	-305.7720	6.8612	25.8275	38.7990	-12.8711	14.9592	-0.2392	151.5367	257.3016	-26.2885	0.2335	-1.2968	0.1731	4.3308
103		16.3150	5.1647	0.7555	0.5240	-370.9332	1.6020	4.0528	31.8943	-47.3453	47.0552	-7.1287	134.6759	27.4059	63.9149	-0.1744	-4.2087	-1.3234	4.9031
119		1.3150	-5.6876	0.1555	-0.2124	-392.3597	8.9167	6.3679	72.2190	98.6360	111.2423	4.9965	80.8134	41.7231	-16.1479	0.2477	1.7410	-1.4001	2.6406
129		11.3150	4.5473	-0.1824	0.0890	-184.5821	12.6035	7.9285	28.6425	68.2139	130.3151	-33.2593	38.1854	7.0779	-28.0403	0.6798	0.5761	-0.3027	3.8651
139		28.3150	6.6465	0.3466	-0.1298	-350.1662	8.8457	9.9694	-1.6063	-39.3698	197.4488	-47.7848	31.1967	-16.6519	13.2784	0.0870	0.6182	-3.0672	7.7527
149		16.3150	5.1647	-0.8445	-0.1499	-214.0392	13.3253	3.1878	4.0448	19.3168	106.7722	-30.7073	-41.6234	316.9091	109.3155	-0.2722	-1.5941	0.7008	7.1760
159		7.3150	4.0533	-0.7128	-0.2239	-411.5070	123.3593	28.1580	-25.7886	-99.2166	-111.3313	-65.5057	-54.0664	274.0644	97.0167	-0.3268	-12.9302	-0.3416	9.7211
169		11.3150	4.5473	-1.9824	-1.1442	-501.5225	129.5946	18.9048	58.9901	-172.0809	-60.0760	-77.8632	-90.3734	51.7804	114.7708	-0.4847	-19.8192	1.6757	12.8493
179		16.3150	5.1647	-1.2445	-1.0684	-529.9412	114.1371	-43.2615	278.3264	-248.7397	62.1727	-78.6159	-84.2628	304.0971	110.2218	-0.7889	-22.3489	0.8951	15.0976
SN Ratio		0.0532	0.0103	0.0072	0.0144	0.0936	0.0255	0.0027	0.0113	0.0018	0.0087	0.0538	0.0003	0.0197	0.0234	0.0002	0.0150	0.0006	
Beta		1.7478	0.4151	-0.0568	-0.0424	-48.6562	6.0562	1.0932	6.8292	-4.0406	6.7947	-4.7485	1.3030	18.9830	6.7624	-0.0061	-0.8148	-0.0275	

(*) Mi = True level of severity

Table 21: Summary of data analysis with 19 variables (2 variables with zero variance)

Abnormal	Mi(*)	U1	U2	U3	U4	U5	U6	U7	U8	U9	U10	U11	U12	U13	U14	U15	U16	U17	U18	U19	YI (predicted)
1	3	0	-5	12.3150	-4.8232	0.5086	-0.0050	-247.2041	5.9966	9.8345	38.4890	53.9519	3.2878	-0.3439	91.0072	218.5704	96.9192	0.5103	3.8723	1.2164	3.4401
2	3	0	-10	16.3150	-5.8111	-0.6521	-0.3753	-339.3995	13.2639	21.7816	3.5642	159.4430	47.6378	25.7567	19.9424	38.6237	46.2383	-0.0509	-0.9670	-0.6080	4.5581
3	3	-3	0	7.3150	-5.6876	-0.5445	-0.3327	-317.0591	0.4772	-2.7434	27.4543	51.3503	3.1881	-0.1598	5.8983	115.8052	36.4650	0.9933	0.8872	0.2391	3.3564
4	3	0	-4	8.3150	4.6707	0.9390	0.0301	-121.7981	7.4455	24.5579	31.1738	53.6886	53.5027	8.1512	51.5605	235.2134	51.7450	0.6046	0.4109	2.1180	3.9019
5	3	-4	0	7.3150	3.3124	0.1555	-0.1327	-222.0592	-2.6516	8.1690	-27.5355	138.1347	114.7010	28.9314	-20.1444	90.6090	21.4934	0.4055	-1.6543	2.2187	5.4607
6	3	-4	0	6.3150	3.8063	-0.0142	0.1228	-174.4202	20.2183	65.1913	10.9267	52.9944	27.4622	7.3102	44.3797	61.9772	61.8750	0.7963	0.5993	3.5203	4.4063
7	3	-4	5	6.3150	2.0775	-0.1205	-0.0104	-189.7995	21.4092	69.3419	17.3681	82.0347	36.8372	15.0119	58.2735	81.3859	106.1382	0.7853	1.9013	3.6687	5.3589
8	3	-4	0	15.3150	5.0412	0.0617	-0.0996	-217.5968	0.0803	11.0121	5.9138	-24.2147	26.4896	2.1381	46.1576	340.1646	99.7916	0.6016	3.2652	3.3896	4.9194
9	3	0	7	10.3150	4.5473	-0.3686	-0.0551	-208.6192	3.1314	30.5279	18.3591	-8.2040	44.8183	18.3955	140.4198	327.9404	87.4870	0.7817	-0.4917	4.4366	5.4957
10	3	0	7	16.3150	2.2010	0.5871	0.7156	-221.5125	1.9417	11.9757	31.8713	32.3709	77.3551	15.0769	128.5416	125.2338	194.5158	0.5961	2.2735	2.5394	5.3191
11	9	0	7	1.3150	-6.4285	0.1099	-0.1937	-379.0782	3.8004	18.6867	69.3825	187.6399	124.2687	54.5396	103.9712	110.3184	88.6731	0.2902	1.7963	-0.4638	6.5812
12	9	-4	7	11.3150	2.2010	-0.3129	0.0748	-72.5950	16.7374	24.9889	30.3079	111.9320	173.9234	28.8658	55.6367	130.8877	50.1456	1.1011	2.4019	4.3666	7.7220
13	9	0	5	28.3150	4.9177	0.2541	0.0171	-210.4862	10.2735	16.2116	-14.0044	-15.2533	222.0768	24.0090	40.3074	119.3488	73.5301	0.6111	0.7587	1.1598	7.5838
14	9	0	-10	16.3150	2.0775	-1.0205	-0.3085	-122.6345	17.0910	23.8848	8.1721	64.6856	144.6806	16.3409	-40.5239	368.8209	75.5318	0.3851	1.9974	3.5958	7.0952
15	9	-5	0	7.3150	2.0775	-0.8205	-0.2677	-308.3187	119.6389	150.9857	34.6156	47.0662	60.0346	6.3440	-69.0617	300.2732	41.4337	0.5561	0.2120	3.1967	7.2938
16	9	0	-10	11.3150	4.6707	-1.9610	-1.3495	-426.0316	125.1581	152.5561	106.4050	9.8985	117.4264	14.7535	-96.3428	45.6021	44.7032	0.5710	-1.0853	4.1349	8.9292
17	9	-6	0	16.3150	4.3003	-1.2838	-1.1606	-429.4657	109.5444	65.6972	335.1143	107.1847	208.8039	51.0812	-54.2971	284.1616	78.3278	0.2070	-3.1676	3.5720	12.3893
SN Ratio		0.014554	5.1E-06	0.0532	0.0031	0.0103	0.0108	0.0692	0.0254	0.0306	0.0131	0.0223	0.1451	0.0545	0.0006	0.0388	0.0288	0.0351	0.0020	0.0384	
Beta		-0.29224	-0.0137	1.7478	0.2319	-0.0664	-0.0443	-37.0105	5.8358	7.3456	8.5277	9.7306	16.3878	3.2332	1.7585	26.0902	9.8617	0.0785	0.0860	0.3718	

(*) Mi = True level of severity

Publications mentioned in the specification are indicative of the levels of those skilled in the art to which the invention pertains. These publications are incorporated herein by reference to the same extent as if each individual publication was specifically and individually incorporated herein by reference.

- 5 The foregoing description is illustrative of particular embodiments of the invention, but is not meant to be a limitation upon the practice thereof. The following claims, including all equivalents thereof, are intended to define the scope of the invention.